LARGE EDDY SIMULATIONS OF FIRE-DRIVEN FLOWS

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ABSTRACT

An approach to the study of gas phase combustion and convection processes in fires using a combination of mathematical analysis and computer simulation is presented. It seeks to solve the governing equations directly (if approximately) by decomposing the fire into a large scale convective and radiative transport problem coupled to a small scale model of combustion and radiative emission. The combustion model assumes that all of the thermodynamic properties of the fluid are tied to the local mixture fraction, which is convected by the large scale motion, which in turn is driven by the heat released by the combustion processes. The large scale flow is studied using finite difference techniques to solve large eddy simulations of the Navier-Stokes equations. The basic theory behind the methodology is outlined and sample results are presented.

INTRODUCTION

Fires have been objects of intense interest throughout history. Despite this interest, it is still not possible to predict quantitatively how a given condensed phase fuel will burn as a function of the given geometric and physical parameters needed to specify a particular scenario. The difficulties associated with analyses of fire phenomena originate with the fact that the active combustion zone of a fire plays two distinct roles which encompass widely different length and time scales. The combustion zone is the region where the local mixing of gasified fuel and air produces the chemical energy release and radiant energy emission that sustains the fire. These processes occur on length scales ranging from a fraction of a millimeter to a few centimeters. At the same time, the combustion zone is a source of buoyancy which induces large scale mixing of air and combustion products, forming a plume which can persist as an organized structure over length scales ranging from a few meters to tens of kilometers, depending on the scenario of interest. The plume in turn, acts as a giant pump that induces a flow pattern throughout the entire structure enclosing an indoor fire. Equally important, the interaction of the large scale mixing and small scale combustion processes creates a combustion zone that is not necessarily small compared with the plume that it generates. Finally, the radiative transport from the entire combustion zone back to the condensed phase fuel surface provides the feedback needed to supply the fire with the fuel required to maintain itself.

Much of the work in fire research concerns the movement of smoke and hot gases in an enclosure. Depending on the scope of the particular scenario, the fire itself is described in relatively simple terms as a source of heat and combustion products [3]. The reason for this is that the fire itself usually occupies a very small fraction of the flow domain, and there is simply not enough spatial resolution to describe fluid motion on length scales at which combustion takes place. Conventional field models using $k - \epsilon$ representations of turbulence often include an empirical description of the combustion processes, but this description relies heavily on the level of turbulence prescribed by the user through the choice of parameters. The approach outlined below, by contrast, seeks approximate solutions to the governing equations directly, by considering combustion, convection, and thermal radiation in parallel, allowing each to evolve separately on its own length and time scale. The complexity of the combustion model which is implemented depends on the spatial and temporal resolution which can be provided by the solution of the Navier-Stokes equations without any empirical turbulence model. Present computational resources allow for two-dimensional simulations with Reynolds numbers approaching 10^5, and three-dimensional calculations approaching 10^4. In the present work, a few 2D, axisymmetric plume simulations will be presented. Simulations in 3D are presently underway, as is the implementation of a soot and radiation model. Before these more elaborate additions are made, however, we seek confirmation that the hydrodynamic model coupled with a simple combustion model adequately describes the flow field.

HYDRODYNAMIC MODEL

We consider a thermally expandable ideal gas with temperature-dependent eddy viscosity and thermal conductivity driven by a prescribed heat source. The motion of the fluid is governed by the equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \tag{1}$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) + \nabla p - \rho \mathbf{g} = \nabla \cdot \boldsymbol{\sigma} \tag{2}$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \frac{dp}{dt} = \dot{q} + \nabla \cdot k \nabla T \tag{3}$$

$$p = \rho \mathcal{R} T \tag{4}$$

Here, all symbols have their usual fluid dynamical meaning: ρ is the density, $\mathbf{u}$ the velocity vector, p the pressure, $\mathbf{g}$ the gravity vector, $\boldsymbol{\sigma}$ the standard viscosity stress tensor, c_p the constant-pressure specific heat, T the temperature, k the thermal conductivity, t the time, $\dot{q}$ the prescribed rate of heat release, and $\mathcal{R}$ the gas constant equal to the difference of the specific heats $\mathcal{R} = c_p - c_v$.

Following the analysis of Rehm and Baum [1], we assume that the flow velocity is much less than the sound speed; the temperature and density variations are large, but the pressure variation small. For an unenclosed buoyant plume, the governing equations may be approximated

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) + \nabla \tilde{p} - \tilde{\rho} \mathbf{g} = \nabla \cdot \boldsymbol{\sigma} \tag{5}$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \dot{q} + \nabla \cdot k \nabla T \tag{6}$$

$$\rho T = \rho_0 T_0 \tag{7}$$

where $\tilde{p}$ is the perturbation of the pressure from hydrostatic, $\tilde{\rho}$ the perturbation of density from the ambient. Because of the removal of the temporal derivative of pressure from the energy equation, there is no explicit equation for the change in pressure with time. To update the velocity components, the pressure gradient must be found by taking the divergence of the momentum equation, yielding an elliptic equation for the pressure

$$\nabla \cdot \frac{1}{\rho} \nabla p = -\nabla \cdot \mathbf{F} - \frac{\partial}{\partial t} \nabla \cdot \mathbf{u} \tag{8}$$

where the term $\mathbf{F}$ includes all the convective and diffusive terms. The divergence $\nabla \cdot \mathbf{u}$ is found by combining Eqs. (1), (3), and (4).

$$\nabla \cdot \mathbf{u} = \frac{\gamma - 1}{\gamma} (\dot{q} + \nabla \cdot k \nabla T) \tag{9}$$

Eq. (8) is a nonseparable elliptic equation which needs to be solved twice at each time step. To make the code run more rapidly, it is assumed that the density in Eq. (8) is ambient. This represents the neglect of the term $(1 - \rho) \nabla p$ from Eq. (5). This term is clearly negligible compared with those retained far from the combustion zone of the plume. Moreover, in the combustion zone, it competes with both the gravitational acceleration and viscous terms in generating vorticity. In fact, unless $\nabla p / \rho_\infty$ generates an acceleration comparable to free fall, it is small compared with the gravitational force even in the combustion zone. Finally, since the velocity field at any point in the combustion zone is influenced by the vorticity field everywhere in the plume, and the expansion velocity in the combustion zone is also large, neglecting this term certainly represents a tolerable error.

The simplified equations above are nondimensionalized, written in cylindrical coordinates, and solved with a finite difference technique. All spatial derivatives are approximated by second-order accurate central differences on a uniform grid, and the solution is advanced in time with a simple Runge-Kutta scheme. The examples below are two-dimensional, axially-symmetric, but the methodology is suitable for two or three spatial dimensions and any coordinate system. The scenario of interest is the flowing of either a hot or a combustible gas from a circular burner at low velocities relative to the characteristic buoyant velocity. The space surrounding the burner is assumed to be open, except for a smooth surface flush with the burner edge (a floor). Simulations are begun by instantaneously rupturing an imaginary membrane covering the burner opening; and in the combustible case ignition is assumed instantaneous as well. First, the case of a noncombusting hot gas will be described, followed by a description of the combustion model and an example for a combusting gas.

NONCOMBUSTION CASE

As a first example of the methodology, consider the buoyant rise of a hot gas from a circular orifice. The initial temperature of the gas is 5 times the ambient temperature. There is a small initial velocity imposed on the gas (the Richardson number is 400), thus the motion is buoyancy driven. An axisymmetric calculation has been carried out for a Reynolds number of 10,000 based on the diameter of the orifice D and the characteristic velocity of the flow $\sqrt{gD}$. Given that the kinematic viscosity of air at room temperature is about 0.15 cm^2/s, this Reynolds number corresponds to an orifice about 13 cm in diameter.

Figure 1 shows the velocity and temperature profile of a typical plume simulation. The structure of the plume is governed by the periodic shedding of toroidal vortices. This shedding is seen as a series of pulsations whose frequency is inversely proportional to the square root of the orifice diameter. Cetegen and Ahmed [4] refined this correlation to show dependence of initial velocity

$$f = K \sqrt{\frac{g}{D}} \left[\left(1 + \frac{1}{\mathrm{Ri}} \right)^{\frac{1}{2}} \frac{1}{\sqrt{\mathrm{Ri}}} \right]^{-1} \tag{10}$$

where K varies between 0.5 and 0.7. The Richardson number, Ri, is defined

$$\mathrm{Ri} = \frac{(\rho_\infty - \rho_f) g D}{\rho_f V_f^2} \tag{11}$$

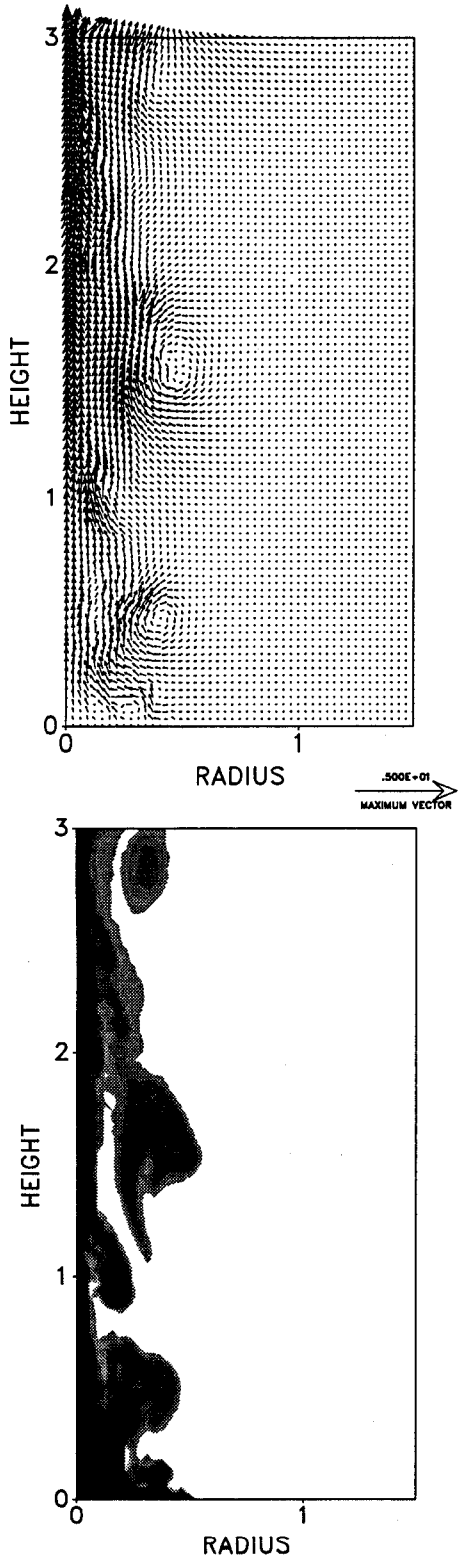

FIGURE 1: VELOCITY AND TEMPERATURE PROFILE OF AN AXISYMMETRIC NONREACTING BUOYANT PLUME.

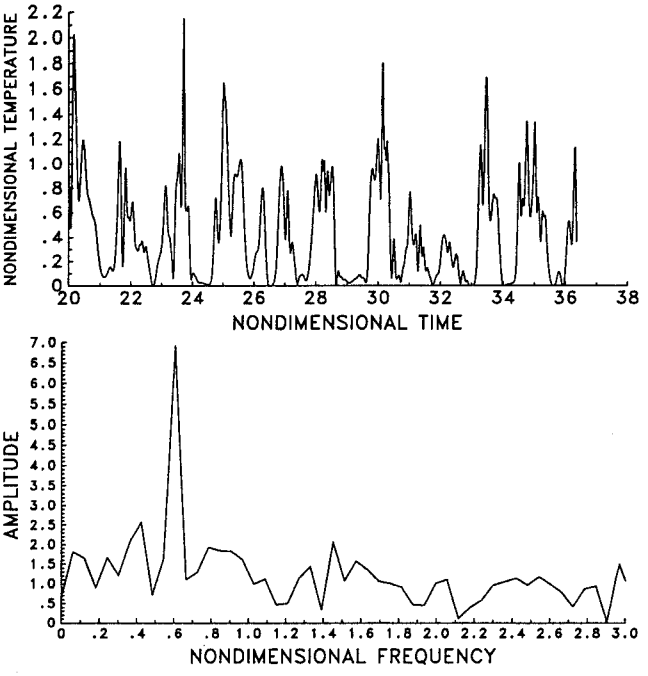

FIGURE 2: NONDIMENSIONALIZED TEMPERATURE HISTORY ABOVE THE BURNER OPENING, FOLLOWED BY THE FREQENCY SPECTRUM.

where ρ_f is the source fluid density, ρ_∞ the ambient air density and V_f the bulk velocity of the gas stream at the source. As a first check on the accuracy of the hydrodynamics, the frequency of the simulated plume pulsations was checked. Figure 2 shows the time history of temperature 0.2 burner diameters above the opening, halfway between the center and the edge. The frequency spectrum reveals a nondimensionalized frequency (which is equivalent to the factor K in Eq. (10)) of about 0.6. The Richardson number is 400. This compares reasonably well with the experimental correlation.

The calculation shown required a grid with 96 cells in the radial direction and 192 cells in the axial. This represents a modest calculation, requiring about 3 hours of CPU time on an IBM/RISC 6000 workstation to simulate about 5 seconds real time. Work is presently underway to compare the temperature and velocity of the simulated plume with available experimental data.

COMBUSTION CASE

The combustion process is idealized as a single global reaction which proceeds at an effectively infinite rate whenever the reactants come into contact [5]. With the assumption of a unity Lewis number and appropriate boundary conditions the mass fractions and temperature can be related to a mixture fraction variable. The mixture fraction, $Z(\vec{r}, t)$, is the solution to equation

$$\rho(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla)Z = \nabla \cdot (\rho D \nabla Z) \qquad (12)$$

which is solved along with the hydrodynamic equations discussed above. The velocity vector $\vec{u}$ can always be decomposed into a solenoidal component $\vec{v}$ and an irrotational component $\nabla\phi$. The solenoidal component is by definition divergence free, while the potential flow carries the expansion of the gas induced by the combustion heat release. This follows from the mass conservation equation which can be written in the form:

$$(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla)\rho + \rho\nabla \cdot \vec{u} = 0 \qquad (13)$$

Since the temperature, and consequently the density, can be expressed as a function of the mixture fraction, combining equations (12) and (13) with the velocity decomposition described above yields the following equation for the potential function:

$$\nabla^2\phi = \frac{d(1/\rho)}{dZ}\nabla \cdot (\rho D \nabla Z) \qquad (14)$$

Equation(14) clearly relates the potential flow to the mixture fraction and hence the combustion heat release. The functional relationship between mixture fraction and density (temperature) can be extracted from experiments [5]. At the moment, a piecewise linear relationship is assumed, requiring the prescription of the temperature of the fuel gas as it exits the burner, the flame temperature, and the value of the mixture fraction which defines the location of the flame.

The direct calculation of the combustion processes would require the solution of the equations of motion including the mixture fraction down to length scales in which the diffusive processes dominate the convective motion. This is not feasible at present, since the active combustion zone of a fire is usually only a small fraction of the space that must be included in any simulation. The use of the fast chemistry approximation in the present paper is an appropriate first step. It is consistent with more detailed mixture fraction based combustion theories currently in use, and it permits the use of experimental data from fire experiments in a way that does not violate the consequences of those theories.

An example of a simulated combusting plume is shown in Fig. 3. In this case, the flame temperature was assumed to be 5 times the ambient, the gas temperature at the burner was assumed to be twice ambient, and the value of the mixture fraction corresponding to the flame sheet location was assumed to be 0.2. These quantities were chosen arbitrarily, with no attempt to represent a given fuel. The flame temperature is not unrealistic if one allows for radiative losses [5]. The intent of the example is merely to demonstrate the implementation of the simple combustion model into the hydrodynamic code. Presently, efforts are underway to compare the simulations to real fires.

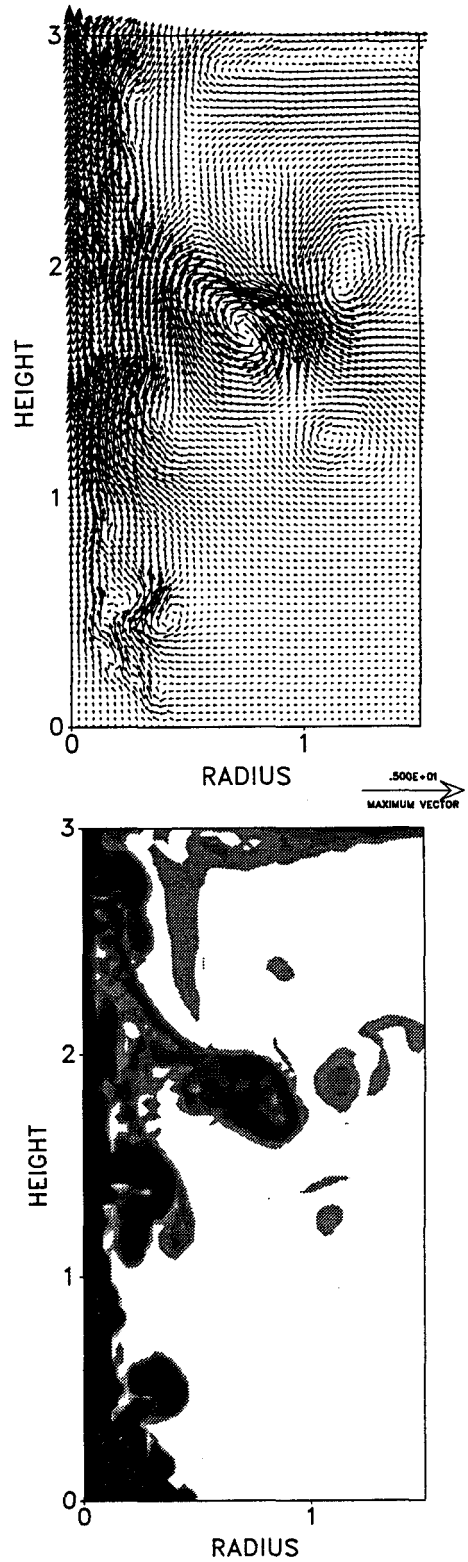

FIGURE 3: VELOCITY AND TEMPERATURE PROFILE OF AN AXISYMMETRIC COMBUSTING BUOYANT PLUME.

CONCLUSION

Experiments are presently being planned to confirm the approach taken in solving the hydrodynamic equations. These would include

spatially and temporally resolved concentration and velocity measurements. Assuming the results for nonreacting plumes compares favorably with the numerical simulations, more elaborate models of combustion, soot production and radiation can then be added. The complexity of these additions will depend on the spatial and temporal resolution which can be achieved in the non-reacting case, which obviously depends on whether the simulation is two or three dimensional.

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